

Phosphonic acid, bis(1-methylethyl) ester
1809-20-7 | DTXSID7061988

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 2.12

Global applicability domain: Inside

Local applicability domain index: 4.68e-01

Confidence level: 7.56e-01

Nearest Neighbors from the Training Set

Image not found

Triethyl phosphate

Measured: 1.29

Predicted: 1.38

Image not found

2,2,4-Trimethyl-1,3-pentanediol

Measured: 1.00

Predicted: 1.47

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Sulfolane

Measured: 7.08

Predicted: 6.91

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1,1'-Oxybis-2-propanol

Measured: 4.57

Predicted: 3.83

Image not found

Trimethyl phosphate

Measured: 1.41

Predicted: 1.50